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14. ABSTRACT The goal of the project was to develop new numerical schemes and solvers for high-order accurate simulations of problems in fluid and solid mechanics. Three main areas were addressed – the high computational cost of existing methods, their lack of robustness, and the need for new high-order mesh manipulation algorithms. The project has led to significant developments in so-called Line-DG and IMEX based numerical schemes, new formulations for problems with deforming domains, artificial viscosity based stabilization, and mesh deformation using a nonlinear elasticity analogy. The results were applied to a number of important real-world problems, such as drag prediction for turbulent flows, flapping flight with fluid-structure interaction, aeroacoustics problems, and transonic/supersonic flow problems. The findings were disseminated through a wide range of publications, presentations, and public domain software.						
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FINAL REPORT

(YIP-10) EFFICIENT AND ROBUST HIGH-ORDER METHODS FOR FLUID AND SOLID MECHANICS

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Abstract

The goal of the project was to develop new numerical schemes and solvers for high-order accurate simulations of problems in fluid and solid mechanics. Three main areas were addressed – the high computational cost of existing methods, their lack of robustness, and the need for new high-order mesh manipulation algorithms. The project has led to significant developments in so-called Line-DG and IMEX based numerical schemes, new formulations for problems with deforming domains, artificial viscosity based stabilization, and mesh deformation using a nonlinear elasticity analogy. The results were applied to a number of important real-world problems, such as drag prediction for turbulent flows, flapping flight with fluid-structure interaction, aeroacoustics problems, and transonic/supersonic flow problems. The findings were disseminated through a wide range of publications, presentations, and public domain software.

Objectives

The goal of the project was to develop new numerical schemes and solvers for high-order accurate simulations of problems in fluid and solid mechanics. Three main areas were addressed – the high computational cost of existing methods, their lack of robustness, and the need for new high-order mesh manipulation algorithms. The project has led to significant developments in so-called Line-DG and IMEX based numerical schemes, new formulations for problems with deforming domains, artificial viscosity based stabilization, and mesh deformation using a nonlinear elasticity analogy. The results were applied to a number of important real-world problems, such as drag prediction for turbulent flows, flapping flight with fluid-structure interaction, aeroacoustics problems, and transonic/supersonic flow problems. The findings were disseminated through a wide range of publications, presentations, and public domain software.

Accomplishments

During the award period, we have conducted several significant research efforts in the general area of high-order accurate numerical methods for solving partial differential equations on unstructured meshes. It is widely believed that these new methods will eventually replace the more traditional simulation techniques for challenging problems in fluid and solid mechanics, for example with propagating waves, turbulent flow, nonlinear interactions, and multiple scales. However, several new developments are required to make high-order methods competitive, such as more efficient numerical solvers and increased robustness. Our work has addressed many of these issues, and below we summarize the research that we have carried out.

The Line Discontinuous Galerkin (Line-DG) Method

In [8, 11], we presented a new line-based discontinuous Galerkin (DG) discretization scheme for first- and second-order systems of partial differential equations. The scheme is based on fully unstructured meshes of quadrilateral or hexahedral elements, and it is closely related to the standard nodal DG scheme as well as several of its variants such as the collocation-based DG spectral element method (DGSEM) or the spectral difference (SD) method. However, our motivation is to maximize the sparsity of the Jacobian matrices, since this directly translates into higher performance in particular for implicit solvers, while maintaining many of the good properties of the DG scheme.

The discretization starts by mapping a first-order system of conservation laws to a reference frame in terms of the contravariant fluxes, see Figure 1. Each of the spatial derivatives is then discretized separately using a standard DG scheme:

$$\begin{aligned} \int_0^1 \mathbf{r}_{jk}(\xi) \cdot \mathbf{v}(\xi) d\xi &= \int_0^1 \frac{d\widetilde{\mathbf{f}}_1(\mathbf{u}_{jk}(\xi))}{d\xi} \cdot \mathbf{v}(\xi) d\xi \\ &= \widehat{\widetilde{\mathbf{f}}_1}(\mathbf{u}_{jk}^+(1), \mathbf{u}_{jk}(1)) \cdot \mathbf{v}(1) - \widehat{\widetilde{\mathbf{f}}_1}(\mathbf{u}_{jk}(0), \mathbf{u}_{jk}^-(0)) \cdot \mathbf{v}(0) - \int_0^1 \widetilde{\mathbf{f}}_1(\mathbf{u}_{jk}(\xi)) \cdot \frac{d\mathbf{v}}{d\xi} d\xi, \end{aligned} \quad (1)$$

where the numerical contravariant fluxes can be written in terms of a standard approximate Riemann solver for the original fluxes, since

$$\widetilde{\mathbf{f}}_1 = \widetilde{\mathbf{F}} \cdot \mathbf{N}_1^+ = (J\mathbf{G}^{-1}\mathbf{F}) \cdot \mathbf{N}_1^+ = \mathbf{F} \cdot (J\mathbf{G}^{-T}\mathbf{N}_1^+) = \mathbf{F} \cdot \mathbf{n}_1^+ \quad (2)$$

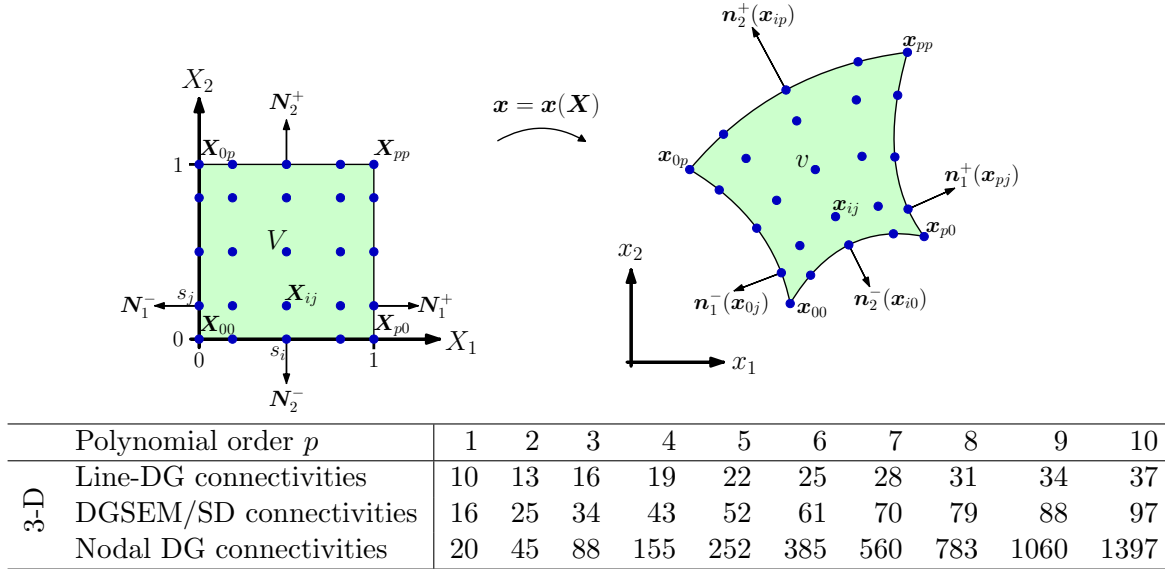


Figure 1: Top: A two-dimensional illustration of the mapping from a reference element V to the actual curved element v , for the case $p = 4$. Bottom: The number of connectivities per node for a first-order operator and 3-D hexahedral elements with the Line-DG, the DGSEM/SD, and the nodal DG methods.

Note that each derivative is essentially a one-dimensional discretization, which results in a very high level of sparsity. The resulting scheme is similar to a collocation scheme, but it uses fully consistent integration along each 1-D coordinate direction which results in different properties for nonlinear problems and curved elements. Also, the scheme uses solution points along each element face, which further reduces the number of connections with the neighboring elements. This sparsity pattern is illustrated in Figure 1 where we note that in three dimensions, already for $p = 3$ the Line-DG method is 5.5 times sparser than nodal DG, and for $p = 10$ it is almost 40 times sparser. This reduction in stencil size translates into lower assembly times, but more importantly, for matrix-based solvers it means drastically lower storage requirements and faster matrix-vector products for iterative implicit solvers. For second-order derivatives, we use an LDG-type scheme with consistent switches along globally connected lines.

The scheme appears well suited for a wide range of problems, and we have demonstrated optimal convergence for viscous and convective model problems, as well as the full compressible Navier-Stokes equations. An example of a turbulent flow is shown in figure 2, where the Line-DG method with ILES modeling is used to predict the acoustic response of a recorder.

Efficient LES Time-Integration using Implicit-Explicit Runge-Kutta Schemes

For many flow problems modeled by Large Eddy Simulation (LES), the computational meshes are such that a majority of the elements would allow for explicit timestepping, but the CFL-condition is limited by the smaller stretched elements in the boundary layers. We have developed an implicit-explicit time-integration scheme that uses an implicit solver only for the smaller portion of the domain where it is required to avoid severe timestep restrictions, but an efficient explicit solver for the rest of the domain [2]. We use the Runge-Kutta IMEX schemes and have demonstrated the stability and accuracy of the solver for a wide range of schemes and orders of accuracy. In addition,

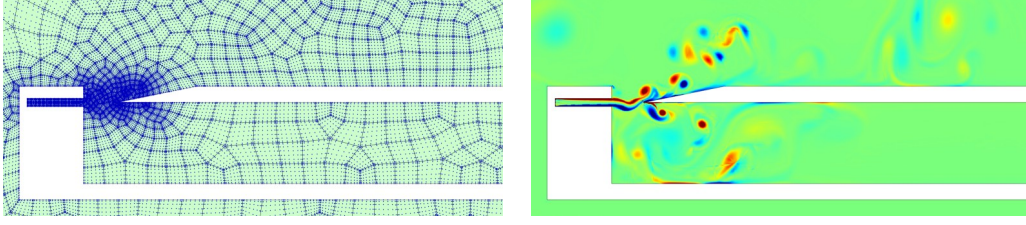


Figure 2: Simulation of the aeroacoustics of a recorder, using the Line-DG scheme and ILES modeling. The left plots show the mesh, with polynomial degrees $p = 7$ within each element, and the right plot shows a sample solution (vorticity).

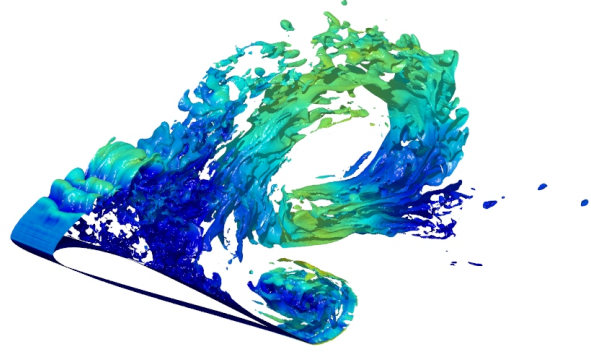
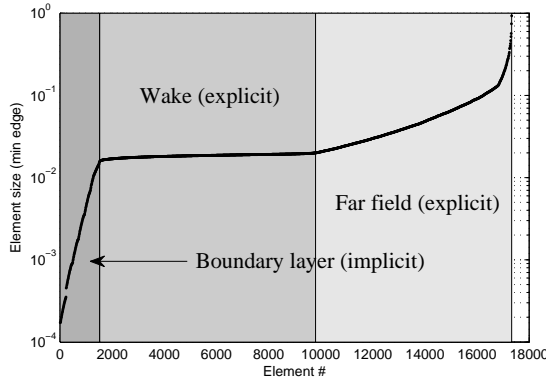


Figure 3: Splitting of the mesh around an SD7003 airfoil into implicit and explicit elements. Less than 9% of the elements are in the boundary layer and integrated using the implicit scheme. The right plot shows an instantaneous flow solution, as isosurfaces of the entropy colored by the Mach number.

we use a quasi-Newton method for the implicit region, which allows us to re-use the Jacobian matrices and their incomplete factorizations for a large number of timesteps. We also showed the application of the technique to a realistic LES-type problem of turbulent flow around an airfoil, where we conclude that the approach can give performance that is superior to both fully explicit and fully implicit methods (see figure 3). The histogram of the elements sizes shows how about 9% of the elements are treated implicitly.

IMEX schemes for Fluid-Structure Interaction

Many important scientific and engineering problems require predictions of fluid-structure interaction (FSI). For example, oscillatory interactions in engineering systems (e.g. aircraft, turbines, and bridges) can lead to failure. The blood flow in arteries and artificial heart valves is highly dependent on structural interactions. These interactions often involve multiple scales and non-linear effects, which makes it challenging to solve even relatively simple problems accurately. In [17, 19], we presented a high-order accurate scheme for fully coupled FSI problems. Using implicit-explicit (IMEX) Runge-Kutta methods, we treat a *predicted* traction $\hat{\mathbf{t}}$ explicitly and everything

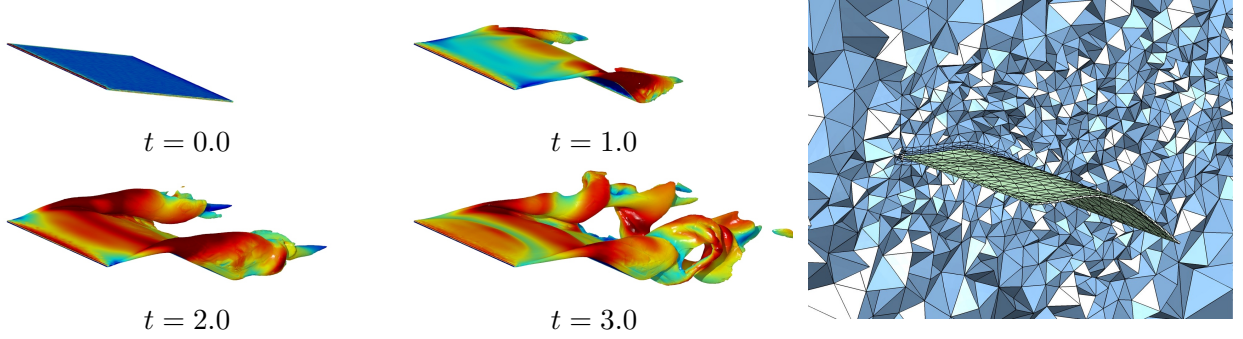


Figure 4: Fluid-structure interaction simulation of the flow around a three dimensional flexible membrane at various times (Mach number on iso-entropy surfaces). Compared to a rigid plate, the leading edge of the membrane aligns with the fluid and reduces the leading edge separation. The right plot shows a sample deformed mesh used in the ALE formulation for the fluid problem.

else implicitly:

$$\mathbf{r} = \begin{bmatrix} \mathbf{r}^f(\mathbf{u}^f; \mathbf{x}(\mathbf{u}^s)) \\ \mathbf{r}^s(\mathbf{u}^s; \mathbf{t}(\mathbf{u}^f)) \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{r}^f(\mathbf{u}^f; \mathbf{x}(\mathbf{u}^s)) \\ \mathbf{r}^s(\mathbf{u}^s; \tilde{\mathbf{t}}) \end{bmatrix}}_{\text{implicit}} + \underbrace{\begin{bmatrix} \mathbf{r}^{fs}(\mathbf{t}(\mathbf{u}^f) - \tilde{\mathbf{t}}) \end{bmatrix}}_{\text{explicit}}$$

where the superscripts f and s correspond to the fluid and the structure, respectively. This leads to a block upper triangular system that fully decouples the implicit solution procedures for the fluid and the solid parts, which we perform using two separate efficient parallel solvers. We also demonstrated using a model problem that subiterations are generally not required, which gives the scheme close to the optimal performance of solving the fluid and structure separately. An example of highly separated flow around a thin membrane is shown in Figure 4.

Artificial viscosity based shock capturing for transient flow problems

We have previously introduced a widely popular artificial viscosity based scheme for sub-cell shock capturing with high-order DG schemes. A highly selective sensor is based on the decay rate of the expansion coefficients of the solution in an orthogonal basis. The scheme is an attractive alternative to limiting, partly because of the subgrid accuracy, the ability to obtain Newton-converged solutions, and the ease of implementation. We have recently continued this work and developed similar schemes for transient problems with moving shocks, time-stepped using high-order accurate implicit schemes with Jacobian-based Newton-Krylov solvers. In [16], we demonstrated that the sensors can be coupled weakly without losing robustness, which simplifies the implementation and reduces the computational times. The weak coupling also allows for non-compact regularization of the artificial viscosity, and we show that C^0 and C^2 regularity in the sensor greatly improves the solution quality. The hypersonic double mach reflection problem of Woodward and Colella is shown in figure 5 (top), as the density field and the applied artificial viscosity. In the bottom plot we show a 3-D problem with the transonic flow around a tapered wing, as pressure and the applied artificial viscosity. In both cases, the plots clearly indicate how the sensor is applied only to a narrow band of elements.

Arbitrary Lagrangian-Eulerian Formulations

Several approaches have been proposed for handling CFD simulations that involve time-varying domains with moving or deformable bodies. One particularly successful method is the Arbitrary

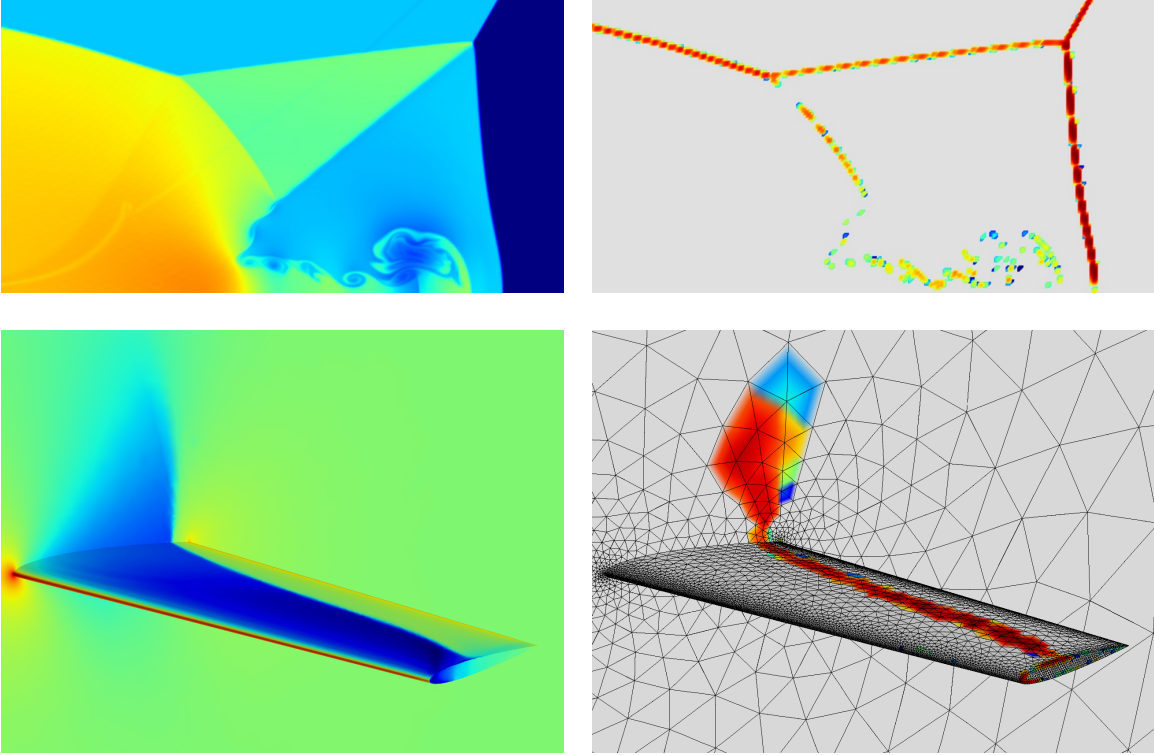


Figure 5: Top: The double-mach reflection problem of Woodward and Colella, showing density (left) and the C^0 -continuous artificial viscosity (right). Bottom: The transonic flow around a tapered wing, pressure (left) and the artificial viscosity (right).

Lagrangian-Eulerian (ALE) formulation, where the mesh is deformed arbitrarily but conforming to the moving boundaries. The physical equations are modified with convective terms to account for the grid motion. We have developed a mapping-based ALE scheme where the modified equations are always solved on a fixed grid. This has the advantage that the scheme is stable and accurate for arbitrary orders of accuracy in space and time. The so-called Geometric Conservation Law (GCL) is handled by solving an additional equations for the Jacobian of the mapping. Using a nonlinear elasticity approach, we can produce mappings for highly stretched and deformed domains, see Figure 6 for an example of a flapping bat and a corresponding flow field. We have also derived so-called stage-consistent mesh velocities for implicit Runge-Kutta schemes [19], which is a general framework for deriving high-order accurate numerical mappings from a set of deformed meshes.

High Fidelity Simulation of Optimized Flapping Wing MAVs

In [3, 7, 14], we proposed a multi-fidelity framework for the design of flapping wing Micro Aerial Vehicles. Since high-fidelity solvers are prohibitively expensive for using in the optimization process, we use a wake-only method and a fast panel code to find candidate designs, which are validated using our high-order Navier-Stokes code. The deforming domain is discretized using our mapping-based ALE approach. The need for high-order methods is clearly seen in our p-convergence studies, where the forces vary substantially with polynomial orders $p = 1$ and $p = 2$ but essentially show grid convergence for $p = 3$ and higher.

In our design study, we found that the designs obtained by the low-fidelity solvers often perform poorly when including the viscous effects of the high-fidelity DG solver, due to the large amounts of

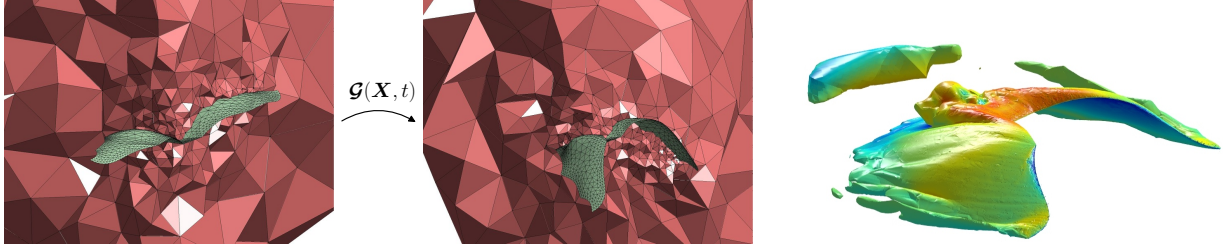


Figure 6: Our high-order mapping-based ALE approach [7, 19] for the simulation of the flapping flight of a bat. The reference mesh (left) is deformed in time using a non-linear elasticity approach which maintains the high-quality of the elements (middle). The right plot shows a sample solution field.

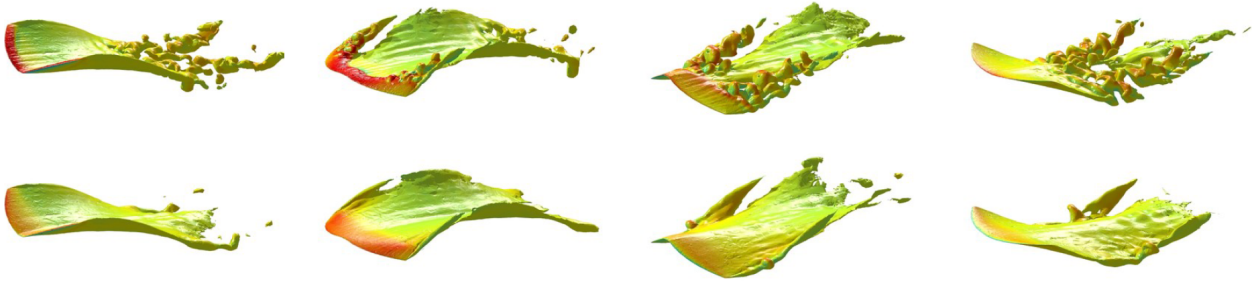


Figure 7: Four snapshots in time of the optimal flapping wing simulation, without camber (top) and with camber (bottom). The flow separation is significantly reduced by using a dynamic cambering.

separation resulting from the wing twisting (Figure 7, top row). To reduce this effect, we introduce a dynamically varying camber along the span, which is aligning the leading edge with the incoming flow. This result in a flow that stays attached for most of the flapping cycle, except for some minor tip vortices, and ultimately a higher performance of the flapping wing pair (Figure 7, bottom row).

Personnel Supported

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Transitions/Interactions

Conference Professional Activities

- Committee member, 22nd International Meshing Roundtable, October 2013
- Mini-symposium organizer, U.S. National Congress on Computational Mechanics, July 2013
- Committee member, 2nd International Workshop on High-Order CFD Methods, May 2013
- Mini-symposium organizer, World Congress of Computational Mechanics, July 2012
- Committee member, 1st International Workshop on High-Order CFD Methods, January 2012

Conference, Colloquia and Workshop Presentations

- AFOSR Computational Mathematics Program Review, July 2013
- 12th U.S. National Congress on Computational Mechanics, July 2013
- 21st AIAA Computational Fluid Dynamics Conference, June 2013
- Drexel University, Math Colloquium, May 2013
- High-Order Nonlinear Numerical Methods for Evolutionary PDEs (HONOM'13), March 2013
- SIAM Computational Science and Engineering, February 2013 (two talks)
- Purdue University, Pure and Applied Mathematics Seminars, November 2012
- AFOSR Computational Mathematics Program Review, August 2012
- World Congress of Computational Mechanics, July 2012
- Lawrence Berkeley National Laboratory, CS Summer Students Seminar, June 2012
- UPC - Universitat Politècnica de Catalunya, DG Summer School, June 2012
- Uppsala University, Scientific Computing Seminar, April 2012
- Uppsala University, Complex System Seminar, April 2012
- 50th AIAA Aerospace Sciences Meeting, January 2012
- Berkeley Optimization Day, October 2011
- UC Berkeley Department of Mathematics Colloquium, September 2011
- 11th U.S. National Congress on Computational Mechanics, July 2011
- ICIAM 2011, July 18, 2011
- AFOSR Computational Mathematics Program Review, June 2011
- 16th Finite Elements in Flow Problems (FEF 2011), March 2011
- Department of EECS, UC Berkeley, March 2011
- SIAM Computational Science and Engineering, March 2011
- NASA Ames Research Center, January 2011
- 49th AIAA Aerospace Sciences Meeting, January 2011

- AFOSR Computational Mathematics Program Review, July 2010

Open-Source Software

- PyDistMesh: A Simple Mesh Generator in Python, at github.com/bfroehle/pydistmesh

New Discoveries, Inventions, or Patent Disclosures

None

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